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Hierarchical Material Models for Fragmentation Modeling in NIF-ALE-AMR

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Abstract.

Fragmentation is a fundamental process that naturally spans micro to macroscopic scales. Recent advances in algorithms, computer simulations, and hardware enable us to connect the continuum to microstructural regimes in a real simulation through a heterogeneous multiscale mathematical model. We apply this model to the problem of predicting how targets in the NIF chamber dismantle, so that optics and diagnostics can be protected from damage. The mechanics of the initial material fracture depend on the microscopic grain structure. In order to effectively simulate the fragmentation, this process must be modeled at the subgrain level with computationally expensive crystal plasticity models. However, there are not enough computational resources to model the entire NIF target at this microscopic scale. In order to accomplish these calculations, a hierarchical material model (HMM) is being developed. The HMM will allow fine-scale modeling of the initial fragmentation using computationally expensive crystal plasticity, while the elements at the mesoscale can use polycrystal models, and the macroscopic elements use analytical flow stress models. The HMM framework is built upon an adaptive mesh refinement (AMR) capability. We present progress in implementing the HMM in the NIF-ALE-AMR code. Additionally, we present test simulations relevant to NIF targets.

1. Introduction

The ultimate goal of this work is to simulate the fragmentation of NIF target assemblies in the aftermath of the laser pulse and ignition. Such simulations will be used to predict fragment sizes and velocities, making it possible to detect larger and faster fragments that have the potential to damage components of the NIF target chamber. This capability will enable the NIF program to verify the design of target assemblies before they are shot and mitigate the risks to the target chamber.

In this paper we present recent progress using the solid material and fracture modeling capability in the NIF ALE-AMR code. This code includes a simple framework for adding local material models relating stress, strain, and various history variables. With the framework the code includes a variety of models including simple isotropic continuum models such as Johnson-Cook, and more complicated anisotropic mesoscale models such as Single Crystal Plasticity. Additionally the code includes a simple void fracture model that allows for fragment formation. Finally, we have begun developing a framework for Hierarchical Material Modeling, which will allow variation of material models at different AMR levels.

2. Simulation Model

NIF ALE-AMR is a continuum finite difference hydrodynamic code derived from an earlier effort at Lawrence Livermore National Laboratory [1]. In this code, the equations are updated in the Lagrangian frame, and can be remapped to the original mesh for Eulerian simulations or some intermediate mesh state for ALE simulations. The code is capable of modeling multiple materials in a single cell by computing material volume fraction, and the material interfaces are tracked through a reconstruction algorithm [2]. All of the field variables are stored using the SAMRAI framework [3] which enables patch based AMR. The ALE capabilities allow the code to more accurately represent motion than an Eulerian code, while avoiding the usual mesh tangling issues in a Lagrangian code. The AMR capability enables the simulation of large domains while refining and spending most of the computational resources where they are needed.

The simulation efforts in this paper focus on the solid material modeling capabilities in NIF ALE-AMR. The material interface in this code has the following form

$$[\sigma_{ij}^{n+1}, e^{n+1}, \mathbf{h}^{n+1}] = f(\sigma_{ij}^{n}, \dot{\epsilon}_{ij}^{n}, e^{n}, \rho^{n}, \mathbf{h}^{n}) \tag{1}$$

which is to say the stress, energy, and material history vector of a cell at the next time step is some function of stress, strain rate, energy, density, and material history vector of that cell at the current state. The material history vector is necessary to store any other persistent data that a material model requires, for instance the level of accumulated damage in models including material failure or the evolving yield stress in J2 plasticity models. In order to tie the full stress tensor into the gas-dynamics equation being solved in NIF ALE-AMR, the equation of motion was updated with an additional stress term

$$\nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla p + \nabla \cdot \Sigma' = 0 \tag{2}$$

where ρ is density, $\mathbf{u}$ is velocity, p is pressure which derives from the trace of the the stress tensor, and Σ' is the deviatoric form of the new stress tensor.

Many of the material models available include some history vector components for tracking material damage and failure. Some of the material models have stress-strain curves that evolve with the amount of damage and all of the damage models have a maximum sustainable damage before material failure and fracture occurs. At this point the material models are silent and a fracture model is required to continue the simulation.

In order to bridge this gap we rely heavily on the NIF ALE-AMR multi-material volume fraction and interface reconstruction algorithms [2]. When the material model in a cell detects failure it is determined whether the cell failed in compression or tension by examining the change in the cell volume. If the cell fails in compression a small volume fraction ($1e^{-6}$) of void material is inserted into the cell. If the material fails in tension a volume fraction of void is introduced to take up the volume gained in the current time step. As cells continue to deform and grow during the simulation the void materials in those cells grow to take up those changes in volume as well. As failures occur in neighboring cells the interface reconstruction algorithm allows the voids to coalesce and form void regions. Finally as these regions spread through the body of the object fragmentation occurs (see Figure 1).

The initial formation of fractures in a material can be heavily influenced by factors in the micro-structure. The AMR capability in the NIF ALE-AMR code allows heavy refinement to occur when conditions approach material fracture. At coarse levels of the AMR mesh every cell contains many material grains, so a continuum material model is well justified. At the finest levels of the AMR mesh the material grains are resolved and a computationally expensive single crystal model is needed. In order to model this variation at different scales, we are developing Hierarchical Material Modeling capabilities. The code has an HMM framework that allows the assignment of different material models at different AMR levels (see Figure 2). This framework

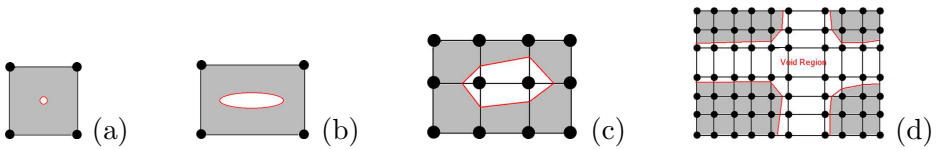

Figure 1. Fracture and fragmentation approach in NIF ALE-AMR. a) Upon material failure in a cell a small volume fraction of void is inserted into the cell. b) As the cell expands in subsequent time steps, the void grows to fill that added space. c) As neighboring cells accumulate void, the interface reconstruction algorithms allow the voids to coalesce and form crack regions. d) Crack regions can grow large enough to span entire cells allowing fragments to form and detach from the material body.

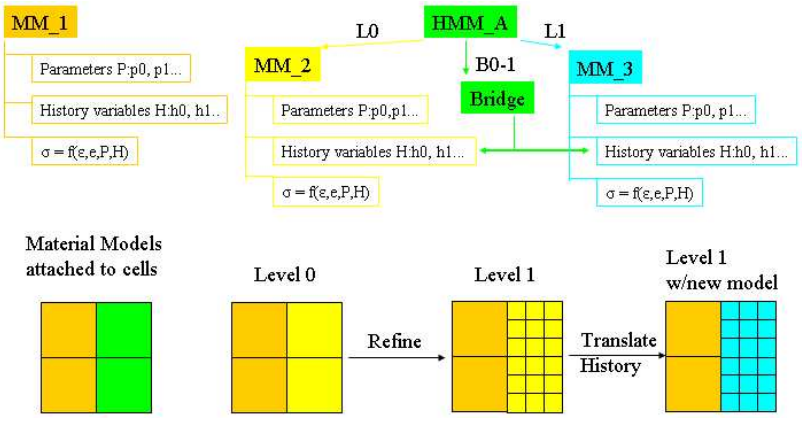

Figure 2. The HMM framework in NIF ALE-AMR

also allows models with dissimilar history variables to be used at different levels by using general including history variable bridging models. This HMM capability will allow us to simulate the micro-structure in large fragmentation problems without requiring expensive micro-structure models everywhere throughout the solid materials.

3. Simulation Results

Plans for the NIF target assembly include two Silicon cooling rings on the outside of the hohlraum. Similarly, the LMJ target assembly includes two Aluminum cooling rings outside of its hohlraum. It is expected that after the hohlraum in either facility absorbs the laser energy it will expand rapidly outward and push on the cooling rings, causing them to fragment and fly outward. We are studying how the choice of material affects the fragment size and velocity of the cooling rings. To begin we simulated an Aluminum ring which is the well quantified ductile material planned for the LMJ cooling rings. This is also pertinent to the NIF cooling rings since fusion experiments will produce neutrons that will heat the NIF Silicon rings and cause them to respond in a more ductile manner. In addition we simulated a Silicon Carbide ring which is a well quantified brittle material similar to the Silicon cooling rings in the NIF plan.

Using the solid materials interface in the NIF ALE-AMR code we simulated the 2D fragmentation of the Aluminum cooling ring and th Silicon Carbide ring with an inner radius of $0.2cm$ and an outer radius of $0.4cm$. An initial velocity of $0.2cm/\mu s$ on the first 2 layers of nodes in the ring to simulate the velocity that the hohlraum will impart after it is vaporized in the NIF shot. For the Aluminum ring, the material model applied was a combination of

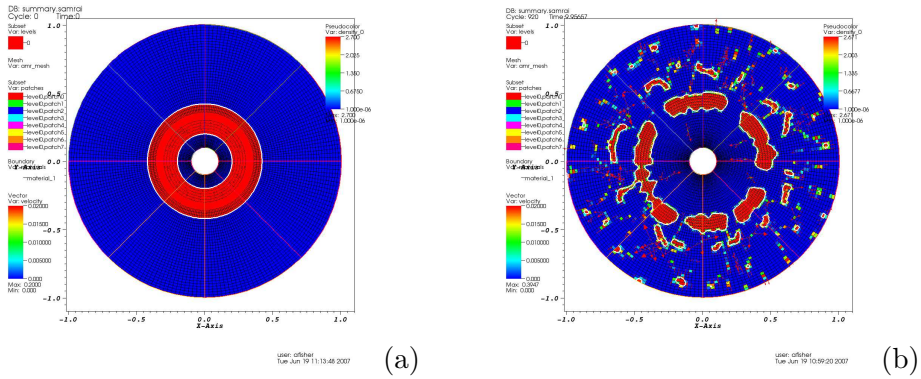

Figure 3. Fragmentation of a expanding cooling rings designs for NIF. a) Expansion of a brittle ring (SiC) b) Expansion of a ductile ring (Al) (Figures will be replaced with data from similar simulations currently running)

isotropic elasticity with J2 plasticity using Johnson-Cook yield strength and failure models. For the Silicon Carbide ring the Johnson-Holmquist 2 model was used. The simulations each ran on 8 processors of LLNL's Zeus computer and took 900 time steps to simulate $10\mu s$ (see Figure 3) (these timings will be updated when currently running simulations finish). These initial 2D simulations indicate that the brittle Silicon Carbide ring forms significantly smaller fragments than the ductile Aluminum ring. One the other hand, the Aluminum ring may be fragmenting into small enough pieces as to not be a major concern. However, further study is warranted.

4. Conclusions and Future Work

The NIF ALE-AMR code has the capability to perform solid material fragmentation simulation work that can mitigate damage risks in the NIF target chamber. This code was used to simulate the fragmentation of potential cooling ring designs in the NIF target assembly. These simulations indicate that brittle materials such as SiC fragment into smaller pieces than ductile materials making them good choices for avoiding damage.

Work in the near future will include simulating the fragmentation of other cooling ring designs including different materials and geometries in 2D and 3D. There are also plans to simulate the fragmentation of other parts of the NIF target assembly. Finally, we are developing a framework for Hierarchical Material Models which will take advantage of the NIF ALE-AMR code's solid modeling capability at the macroscale and the mesoscale and can begin connecting them through AMR.

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